

```
chain nodes : 22 23 24 25 27 28 29 31 34
ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
ring/chain nodes:
    30 32 33
chain bonds :
    3-24 10-27 12-25 17-23 18-22 27-28 29-30 32-33 33-34
ring bonds :
    1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16 12-13 13-14 13-21 15-16 15-20 15-21 16-17 17-18 18-19 19-20
exact/norm bonds :
    1-2 1-6 2-3 3-4 3-24 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16 12-13 12-25 13-14 13-21 15-21 17-23 18-22 27-28 29-30 32-33 33-34
exact bonds :
    10-27
normalized bonds : 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
    containing 1:
G1:H,CH3
```

G2:H,OH,[*1],[*2],[*3]

Match level:
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS
Generic attributes:
 31:

Saturation : Unsaturated

=> s l1 sss full FULL SEARCH INITIATED 13:27:05 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 674 TO ITERATE

100.0% PROCESSED 674 ITERATIONS

162 ANSWERS

SEARCH TIME: 00.00.01

L3 162 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 170.75 171.23

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:27:13 ON 30 APR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 30 Apr 2004 VOL 140 ISS 19 FILE LAST UPDATED: 29 Apr 2004 (20040429/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 22 L3

=> d l4 1-22 bib abs hitstr

L4 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:765217 CAPLUS

DN 138:14135

TI A Solid-Supported, Enantioselective Synthesis Suitable for the Rapid Preparation of Large Numbers of Diverse Structural Analogues of (-)-Saframycin A

AU Myers, Andrew G.; Lanman, Brian A.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

Ι

SO Journal of the American Chemical Society (2002), 124(44), 12969-12971 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:14135

GΙ

AB A 10-step solid-supported, enantioselective synthesis suitable for the rapid preparation of large nos. of diverse structural analogs of saframycin A is described. The synthetic route, which bears analogy to solid-phase peptide synthesis, involves the directed condensation of N-protected $\alpha\text{-amino}$ aldehyde reactants, e.g. N-Fmoc-glycinal (Fmoc = 9-fluorenylmethoxycarbonyl). A novel dual linker, (S)-2-[4-(tertbutyldimethylsilyloxy) -1-butyl]morpholine, was developed for attachment of intermediates to the solid support via a C-protective group, a substituted morpholino nitrile derivative The route employs a novel diastereospecific cyclorelease mechanism, supports structural variation at multiple sites in the saframycin core, and obviates the need for chromatog. purification of the products or any intermediate. To demonstrate the feasibility of structural variation at multiple sites, a matrix of 16 saframycin A analogs, e.g. I, was prepared by parallel synthesis with simultaneous variation of two sites. This work is notable not only as a preliminary step toward large-scale library construction but also as an example of the use of sequential stereoselective C-C bond-forming reactions on the solid phase for the preparation of natural product analogs.

IT 253329-76-9P 429687-34-3P 429687-39-8P 477566-56-6P 477566-57-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of (-)-saframycin A analogs via solid-supported combinatorial chemical using a directed condensation of N-protected amino

CN

aldehydes with (silyloxybutyl)morpholine dual linker and Pictet-Spengler cyclization)

RN 253329-76-9 CAPLUS

Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

429687-34-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16trimethyl-9-pentyl-, (6S,7R,9S,14aS,15R)- (9CI) (CA INDEX NAME)

RN

Absolute stereochemistry.

RN 429687-39-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477566-56-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-[(acetyloxy)methyl]-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 477566-57-7 CAPLUS

CN Propanethioic acid, 2,2-dimethyl-, S-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     2002:391711 CAPLUS
DN
     136:401914
TI
     Preparation of saframycin analogs for pharmaceutical use in the treatment
     of cancer
     Myers, Andrew; Plowright, Alleyn T.; Kung, Daniel W.; Lanman, Brian;
IN
     Barbay, Joseph; Xing, Chengquo
PA
     President and Fellows of Harvard College, USA
     PCT Int. Appl., 203 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
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PΙ
     WO 2002040477
                       A2
                            20020523
                                            WO 2001-US47399
                                                             20011105
     WO 2002040477
                       A3
                            20030227
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
             UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2002039565
                       A5
                            20020527
                                           AU 2002-39565
                                                             20011105
     US 2003008873
                       A1
                            20030109
                                           US 2001-11466
                                                             20011105
     EP 1339713
                       A2
                            20030903
                                           EP 2001-987338
                                                             20011105
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI US 2000-245888P
                      P
                            20001103
     WO 2001-US47399
                            20011105
                       W
OS
     MARPAT 136:401914
GΙ
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AB Saframycin analogs, such as I [R = H, alkyl, acyl, arylacyl, heteroarylacyl, carboxy, arylsulfonyl, etc.], were prepared for therapeutic use as antitumor agents. Thus, I (R = 2-furanylmethyl) was prepared in 95% yield via condensation of 2-furancarboxaldehyde with the corresponding amine I (R = NH2) using sodium triacetoxyborohydride in MeCN. The amine I (R = H) was prepared via a stereoselective sequence of solid phase synthetic steps. The prepared saframycin analogs were assayed for cancer cell growth inhibition of A375 malignant melanoma and A-459 lung carcinoma cell lines.

IT 253329-80-5P 349103-40-8P 429687-32-1P

Ι

Page 6

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of saframycin analogs for pharmaceutical use in the treatment of cancer)

RN 253329-80-5 CAPLUS

CN Propanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-40-8 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 429687-32-1 CAPLUS

CN 2-Quinolinecarboxamide, 6-(4-aminobutoxy)-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 9H-fluoren-9-ylmethyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

RN 349103-36-2 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 349103-37-3 CAPLUS

CN 2-Pyridinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-39-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-,(6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 349103-41-9 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-7-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-42-0 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-methoxy- (9CI) (CA INDEX NAME)

RN 349103-43-1 CAPLUS

CN 2-Quinolinecarboxamide, 6-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-44-2 CAPLUS

CN 2-Quinoxalinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-48-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,
9-[[(2-furanylmethyl)amino]methyl]-6,7,9,14,14a,15-hexahydro-1,10dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-49-7 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,
6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-[[(phenylmethyl)amino]methyl]-, (6S,7R,9R,14aS,15R)- (9CI)
(CA INDEX NAME)

RN 349103-50-0 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-51-1 CAPLUS

CN Benzeneacetamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-52-2 CAPLUS

CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-53-3 CAPLUS

CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 4-methoxyphenyl ester (9CI) (CA INDEX NAME)

RN 349103-54-4 CAPLUS

CN Urea, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-55-5 CAPLUS

CN Benzenesulfonamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 349103-56-6 CAPLUS

CN Carbamic acid, [(1S)-2-[[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-57-7 CAPLUS

CN 1H-Indole-3-propanamide, α-amino-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, (αS)- (9CI) (CA INDEX NAME)

RN 349103-58-8 CAPLUS

CN 1H-Indole-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-59-9 CAPLUS

CN Benzenepropanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-α-oxo- (9CI) (CA INDEX NAME)

RN 349103-60-2 CAPLUS

CN 2-Furancarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-61-3 CAPLUS

CN 1-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-62-4 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2,3,4,5,6-pentafluoro-(9CI)(CA INDEX NAME)

Absolute stereochemistry.

RN 349103-63-5 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-64-6 CAPLUS

CN Propanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-65-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-[[(2-pyridinylmethyl)amino]methyl]-, (6S,7R,9R,14aS,15R)-(9CI) (CA INDEX NAME)

RN 349103-66-8 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-67-9 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-iodo-(9CI) (CA INDEX NAME)

RN 349103-68-0 CAPLUS

CN Benzamide, 2-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-69-1 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-methyl- (9CI) (CA INDEX NAME).

RN 349103-70-4 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-71-5 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-nitro- (9CI) (CA INDEX NAME)

RN 349103-72-6 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-73-7 CAPLUS

CN Benzamide, 4-bromo-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-74-8 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2,6-difluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-75-9 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3,4,5-trimethoxy- (9CI) (CA INDEX NAME)

RN 349103-76-0 CAPLUS

CN 2-Pyridinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-77-1 CAPLUS

CN Pyrazinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-78-2 CAPLUS

CN 1H-Indole-3-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-79-3 CAPLUS

CN 1H-Indole-4-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-80-6 CAPLUS

CN 1H-Indole-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-81-7 CAPLUS

CN 1H-Indole-3-acetamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-α-oxo- (9CI) (CA INDEX NAME)

RN 349103-82-8 CAPLUS CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-[(5,7-dihydro-5,7-dioxo-6H-pyrrolo[3,4-b]pyridin-6-yl)methyl]-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16trimethyl-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-83-9 CAPLUS CN 2-Propenamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 349103-84-0 CAPLUS

CN 1-Naphthalenecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-85-1 CAPLUS

CN 1-Naphthalenecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 349103-86-2 CAPLUS

CN 1-Isoquinolinecarboxamide, 4-bromo-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-87-3 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-

hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-88-4 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methoxy- (9CI) (CA INDEX NAME)

RN 349103-89-5 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-90-8 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-hydroxy- (9CI) (CA INDEX NAME)

RN 349103-91-9 CAPLUS

CN 2-Quinolinecarboxamide, 6-butoxy-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-92-0 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-93-1 CAPLUS

CN 2-Quinolinecarboxamide, 7-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-

6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-94-2 CAPLUS

CN 2-Quinolinecarboxamide, 6-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy-(9CI) (CA INDEX NAME)

RN 349103-95-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-1,2,3,4-tetrahydro-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-28-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-[[bis(2-pyridinylmethyl)amino]methyl]-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-29-6 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7S,9R,14aS,15R)-6,7,9,14,14a,15-hexahydro-1,7,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-30-9 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7S,9R,14aS,15R)-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,7,11,13-pentamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-31-0 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,9R,14aS,15R)-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-33-2 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-[4-[[6-[[6-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-1-oxohexyl]amino]-1-oxohexyl]amino]butoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 429687-34-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-pentyl-, (6S,7R,9S,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-35-4 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-[4-[[6-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1-oxohexyl]amino]butoxy]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 429687-36-5 CAPLUS

CN 2-Pyridinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-hydroxy-5-methyl-(9CI) (CA INDEX NAME)

RN 429687-37-6 CAPLUS

CN 1-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 429687-38-7 CAPLUS

CN 2-Quinolinecarboxamide, N-[[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 429687-39-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 349103-35-1P 429687-78-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of saframycin analogs for pharmaceutical use in the treatment of cancer)

RN 349103-35-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-(aminomethyl)-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 429687-78-5 CAPLUS

CN Carbamic acid, [4-[[2-[[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]amino]carbonyl]-6-quinolinyl]oxy]butyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

Me_

IT 429687-40-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of saframycin analogs for pharmaceutical use in the treatment of cancer)

RN 429687-40-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-[(1E)-2-phenylethenyl]-, (6S,7R,9S,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

- L4 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2002:381108 CAPLUS
- DN 137:182177
- TI Transcriptional response pathways in a yeast strain sensitive to saframycin A and a more potent analog: evidence for a common basis of activity
- AU Plowright, Alleyn T.; Schaus, Scott E.; Myers, Andrew G.
- CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
- SO Chemistry & Biology (2002), 9(5), 607-618 CODEN: CBOLE2; ISSN: 1074-5521
- PB Cell Press
- DT Journal
- LA English

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Saframycin A (I) is a natural product that inhibits human cancer cell proliferation. Its synthetic analog, QAD (II), is a more potent inhibitor of these cells. I does not affect wild-type yeast, but it does inhibit growth of the strain CCY333 (ΔPDR1/PDR3/ERG6) (IC50 = 0.9 μM).

 II is also a more effective inhibitor of CCY333 growth (IC50 = 0.4 μM). Transcription profiling of I- and II-treated CCY333 cultures showed that both drugs generated nearly identical profiles, with altered expression levels (≥2-fold) of >240 genes. Both agents induced the overexpression of genes involved in glycolysis, oxidative stress, and protein degradation and repressed genes encoding histones, biosynthetic enzymes, and the cellular import machinery. Significantly, neither drug affected the expression of known DNA-damage repair genes, as might have been expected if their primary mechanism of action involved the covalent modification of DNA.
- IT 349103-40-8
 - RL: BSU (Biological study, unclassified); BIOL (Biological study) (transcriptional response pathways in a yeast strain sensitive to saframycin A and a more potent analog: evidence for a common basis of activity)
- RN 349103-40-8 CAPLUS
- CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
L4
AN
     2001:545697 CAPLUS
DN
     135:137633
ΤI
     Preparation of saframycin-ecteinascidin analogs and their therapeutic
     applications
IN
     Danishefsky, Samuel J.; Zhou, Bishan
PA
     The Trustees of Columbia University in the City of New York, USA
SO
     PCT Int. Appl., 115 pp.
     CODEN: PIXXD2
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AB Compds. of the saframycin-ecteinascidin series such as I [R1,R4 = H, alkyl, acyl; R3 = =0, OH, ether, sulfide, acyl group such as OC(0)Me, OC(0)Bn and OC(0)Et; R5 = H, halogen, OH, ether, acyl, amide; R6 = =0, OH, OMe, CN, acyloxy; R7 = =0, OH, halogen, ether, acyl; R8 and R9 independently = H, Me, OMe, OEt, CF3, Br, F; R8R9 = OCH2O, five or six membered ring; R10,R11 = Me, OMe, OEt, SMe, SEt; R12 = H, alkyl, acyl; chiral center marked * has the R or the S configuration], were prepared for use as antitumor and antimicrobial agents. Thus, saframycin analog II was prepared via a multistep synthetic sequence starting from 2,4-Dimethoxy-3-methylbenzaldehyde, bromoacetal, 2-hydroxy-4-methoxy-3-methylbenzaldehyde and [[(2E)-4-bromo-2-butenyl]oxy](1,1-dimethylethyl)dimethylsilane. Ecteinascidin 743 I (R1 = Ac, R2R3 = X, R4 = R5 = R7 = H, R6 = α-OH, R8R9 = OCH2O, R10-R12 = Me) was tested for cytotoxicity and antimicrobial activity.

IT 351378-59-1P 351378-84-2P 351378-93-3P

RL: PNU (Preparation, unclassified); PREP (Preparation) (attempted synthesis of)

RN 351378-59-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-9-(hydroxymethyl)-1,2,10,11,13-pentamethoxy-3,12,16trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 351378-84-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-93-3 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

IT 351377-83-8P 351377-84-9P 351377-85-0P 351377-86-1P 351377-88-3P 351378-45-5P 351379-85-6P 351379-86-7P 351379-88-9P 351379-89-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 351377-83-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(acetyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-84-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-85-0 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14aR,15R)-6,7,9,14,14a,15-hexahydro-

13-hydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7,14-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-86-1 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14R,14aR,15R)-6,7,9,14,14a,15-hexahydro-13,14-dihydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7-oxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-88-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 351378-45-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351379-85-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

RN 351379-86-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351379-88-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,
4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

RN 351379-89-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT
     271578-62-2P 273720-76-6P 351377-77-0P
     351377-78-1P 351377-79-2P 351377-81-6P
     351378-24-0P 351378-26-2P 351378-28-4P
     351378-30-8P 351378-32-0P 351378-43-3P
     351378-57-9P 351378-78-4P 351379-71-0P
     351379-73-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of saframycin-ecteinascidin analogs and their therapeutic
        applications)
RN
     271578-62-2 CAPLUS
     6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,
CN
     14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-
     [(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)
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RN 273720-76-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-77-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

RN 351377-78-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351377-79-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-13,14-dihydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14R,14aR,15R)- (9CI) (CA INDEX NAME)

RN 351377-81-6 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-24-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,
14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-1-(phenylmethoxy)9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-26-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 351378-28-4 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-9-(hydroxymethyl)-2,10,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-30-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,
14a,15-dihydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 351378-32-0 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-1,13,14-trihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-43-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 351378-57-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351378-78-4 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

RN 351379-71-0 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 351379-73-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,(6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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AN 2001:327067 CAPLUS

DN 135:92769

TI Synthesis and Evaluation of Bishydroquinone Derivatives of (-)-Saframycin A: Identification of a Versatile Molecular Template Imparting Potent Antiproliferative Activity

AU Myers, Andrew G.; Plowright, Alleyn T.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SO Journal of the American Chemical Society (2001), 123(21), 5114-5115 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 135:92769

GI

AB Saframycin A derivs. (I) were prepared and evaluated for antiproliferative activity against the human cancer cell lines A375 melanoma and A549 lung carcinoma.

Ι

IT 349103-56-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and antiproliferative activity of bishydroquinone derivs. of saframycin A)

RN 349103-56-6 CAPLUS

CN Carbamic acid, [(1S)-2-[[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

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IT
     253329-80-5P 349103-36-2P 349103-37-3P
     349103-38-4P 349103-39-5P 349103-40-8P
     349103-41-9P 349103-42-0P 349103-43-1P
     349103-44-2P 349103-45-3P 349103-48-6P
     349103-49-7P 349103-50-0P 349103-51-1P
     349103-52-2P 349103-53-3P 349103-54-4P
     349103-55-5P 349103-57-7P 349103-58-8P
     349103-59-9P 349103-60-2P 349103-61-3P
     349103-62-4P 349103-63-5P 349103-64-6P
     349103-65-7P 349103-66-8P 349103-67-9P
     349103-68-0P 349103-69-1P 349103-70-4P
     349103-71-5P 349103-72-6P 349103-73-7P
     349103-74-8P 349103-75-9P 349103-76-0P
     349103-77-1P 349103-78-2P 349103-79-3P
     349103-80-6P 349103-81-7P 349103-82-8P
     349103-83-9P 349103-84-0P 349103-85-1P
     349103-86-2P 349103-87-3P 349103-88-4P
     349103-89-5P 349103-90-8P 349103-91-9P
     349103-92-0P 349103-93-1P 349103-94-2P
    349103-95-3P 349103-96-4P 349103-97-5P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); BIOL (Biological
    study); PREP (Preparation)
        (synthesis and antiproliferative activity of bishydroquinone derivs. of
        saframycin A)
RN
    253329-80-5 CAPLUS
CN
    Propanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-
    1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-
    isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-oxo- (9CI) (CA INDEX NAME)
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RN 349103-36-2 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-37-3 CAPLUS

CN 2-Pyridinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-hydroxy- (9CI) (CA INDEX NAME)

RN 349103-38-4 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-hydroxy-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-39-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,
 9-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-6,7,9,14,14a,15 hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-,
 (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 349103-40-8 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-41-9 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-7-methyl- (9CI) (CA INDEX NAME)

RN 349103-42-0 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-43-1 CAPLUS

CN 2-Quinolinecarboxamide, 6-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-44-2 CAPLUS

CN 2-Quinoxalinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-45-3 CAPLUS

CN 2-Quinolinecarboxamide, N-[2-[(6S,7R,9S,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 349103-48-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,
9-[[(2-furanylmethyl)amino]methyl]-6,7,9,14,14a,15-hexahydro-1,10dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-49-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,
6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-[[(phenylmethyl)amino]methyl]-, (6S,7R,9R,14aS,15R)- (9CI)
(CA INDEX NAME)

RN 349103-50-0 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-51-1 CAPLUS

CN Benzeneacetamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-52-2 CAPLUS

CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, phenylmethyl ester (9CI) (CAINDEX NAME)

Absolute stereochemistry.

RN 349103-53-3 CAPLUS

CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 4-methoxyphenyl ester (9CI) (CA INDEX NAME)

RN 349103-54-4 CAPLUS

CN Urea, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-55-5 CAPLUS

CN Benzenesulfonamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 349103-57-7 CAPLUS

CN 1H-Indole-3-propanamide, α -amino-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-58-8 CAPLUS

CN 1H-Indole-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-59-9 CAPLUS

CN Benzenepropanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-α-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-60-2 CAPLUS

CN 2-Furancarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-61-3 CAPLUS

CN 1-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-62-4 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2,3,4,5,6-pentafluoro-(9CI)(CA INDEX NAME)

RN349103-63-5 CAPLUS

Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-CNdihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5Hisoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

349103-64-6 CAPLUS
Propanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-CN1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5Hisoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-65-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-9-[[(2-pyridinylmethyl)amino]methyl]-, (6S,7R,9R,14aS,15R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-66-8 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-67-9 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-iodo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-68-0 CAPLUS

CN Benzamide, 2-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-69-1 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-70-4 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-fluoro- (9CI) (CA INDEX NAME)

RN 349103-71-5 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-nitro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-72-6 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 349103-73-7 CAPLUS

CN Benzamide, 4-bromo-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-74-8 CAPLUS

CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2,6-difluoro-(9CI) (CA INDEX NAME)

RN 349103-75-9 CAPLUS
CN Benzamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3,4,5-trimethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-76-0 CAPLUS

CN 2-Pyridinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-77-1 CAPLUS

CN Pyrazinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-78-2 CAPLUS

CN 1H-Indole-3-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-79-3 CAPLUS

CN 1H-Indole-4-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-80-6 CAPLUS

CN 1H-Indole-2-carboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-5-fluoro-(9CI) (CA INDEX NAME)

RN 349103-81-7 CAPLUS

CN 1H-Indole-3-acetamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-α-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-82-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-[(5,7-dihydro-5,7-dioxo-6H-pyrrolo[3,4-b]pyridin-6-yl)methyl]-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16trimethyl-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RN 349103-83-9 CAPLUS

CN 2-Propenamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 349103-84-0 CAPLUS

CN 1-Naphthalenecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-85-1 CAPLUS

CN 1-Naphthalenecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-86-2 CAPLUS

CN 1-Isoquinolinecarboxamide, 4-bromo-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

RN 349103-87-3 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-88-4 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-89-5 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 349103-90-8 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-91-9 CAPLUS

CN 2-Quinolinecarboxamide, 6-butoxy-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-92-0 CAPLUS

CN 2-Quinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-6-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-93-1 CAPLUS

CN 2-Quinolinecarboxamide, 7-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-94-2 CAPLUS

CN 2-Quinolinecarboxamide, 6-chloro-N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-95-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-1,2,3,4-tetrahydro-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-96-4 CAPLUS

CN 1-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-1,2,3,4-tetrahydro-, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 349103-97-5 CAPLUS

CN 1-Isoquinolinecarboxamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-1,2,3,4-tetrahydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 349103-35-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis and antiproliferative activity of bishydroquinone derivs. of
 saframycin A)

RN 349103-35-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 9-(aminomethyl)-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13tetramethoxy-3,12,16-trimethyl-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2000:577750 CAPLUS
- DN 133:322029
- TI One-Step Construction of the Pentacyclic Skeleton of Saframycin A from a "Trimer" of α -Amino Aldehydes
- AU Myers, Andrew G.; Kung, Daniel W.
- CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
- SO Organic Letters (2000), 2(19), 3019-3022 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 133:322029

GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB The entire skeleton of the saframycin antitumor antibiotics is assembled in one remarkable transformation (I) to (II) from an N-linked oligomer of three α -amino aldehyde components, a reaction pathway that may parallel the biosynthetic route to the saframycins.
- IT 302585-91-7P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (one-step construction of the pentacyclic skeleton of saframycin A from α -amino aldehydes)
- RN 302585-91-7 CAPLUS
- CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12-dimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

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RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:248566 CAPLUS

DN 133:30850

TI A novel face specific Mannich closure providing access to the saframycin-ecteinascidin series of piperazine based alkaloids

AU Zhou, Bishan; Guo, Jinsong; Danishefsky, Samuel J.

CS The Department of Chemistry, Columbia University, New York, NY, 10027, USA

SO Tetrahedron Letters (2000), 41(13), 2043-2046 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:30850

GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB The Mannich-like closure of I to II directly provides the backbone stereochem. required for the titled alkaloids, in contrast to the stereochem. outcome in a related earlier case.

IT 271578-62-2P

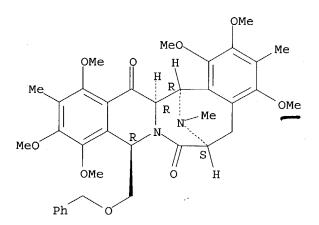
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(face specific Mannich closure providing access to saframycin-ecteinascidin series of piperazine based alkaloids)

RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 273720-76-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (face specific Mannich closure providing access to saframycinecteinascidin series of piperazine based alkaloids)

RN 273720-76-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:248565 CAPLUS

DN 133:4840

TI Synthetic explorations in the saframycin-ecteinascidin series: construction of major chiral subunits through catalytic asymmetric induction

AU Zhou, Bishan; Edmondson, Scott; Padron, Juan; Danishefsky, Samuel J.

CS The Department of Chemistry, Columbia University, New York, NY, 10027, USA

Tetrahedron Letters (2000), 41(13), 2039-2042 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:4840

GI

SO

Same as DNS. 7

AB The major subunits (I and II) needed to reach the titled targets have been assembled by chemical, which included p-Claisen rearrangement, asym. epoxidn. and asym. dihydroxylation.

IT 271578-62-2P

RL: PNU (Preparation, unclassified); PREP (Preparation) (construction of major chiral saframycin subunits via catalytic asym. induction)

RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:705507 CAPLUS

DN 132:64439

TI A Concise, Stereocontrolled Synthesis of (-)-Saframycin A by the Directed Condensation of α -Amino Aldehyde Precursors

AU Myers, Andrew G.; Kung, Daniel W.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SO Journal of the American Chemical Society (1999), 121(46), 10828-10829 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 132:64439

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AB (-)-Saframycin A was prepared in 15% overall yield in 8 steps from the α -amino aldehyde precursors I and II.

IT 253329-76-9P 253329-80-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(stereocontrolled synthesis of (-)-saframycin A by directed condensation of α -amino aldehyde precursors)

RN 253329-76-9 CAPLUS

CN Carbamic acid, [[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

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RN

253329-80-5 CAPLUS
Propanamide, N-[[(6S,7R,9R,14aS,15R)-7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-CNisoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:741636 CAPLUS

DN 123:313604

TI Synthesis of saframycins. X. Transformation of (-)-saframycin A to (-)-saframycin Mx type compound with the structure proposed for saframycin E

AU Saito, Naoki; Harada, Shunji; Nishida, Masayo; Inouye, Izumi; Kubo, Akinori

CS Meiji College Pharmacy, Tokyo, 154, Japan

SO Chemical & Pharmaceutical Bulletin (1995), 43(5), 777-82 CODEN: CPBTAL; ISSN: 0009-2363

PB Pharmaceutical Society of Japan

DT Journal

LA English

AB Treatment of (-)-saframycin A with selenium oxide in acetic acid afforded (-)-saframycin G, and a catalytic reduction and regionelective oxidation sequence

afforded the saframycin Mx type compound We applied this methodol. to the transformation of (\pm) -5-hydroxysaframycin B to the hydroquinone saframycin E. Acetylation of saframycin E with acetic anhydride in pyridine gave the triacetate, which is identical with the triacetyl derivative of natural saframycin E.

IT 160952-79-4P 169616-80-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(transformation of saframycin A to saframycin Mx type compound and total synthesis of saframycin E)

RN 160952-79-4 CAPLUS

CN Propanamide, N-[(7-cyano-6,7,9,14,14a,15-hexahydro-1,4,5,10,13-pentahydroxy-2,11-dimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, [5S-(5 α ,6 α ,7 α ,9.bet a.,14a α ,15 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 169616-80-2 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,4,5,10,13-pentahydroxy-2,11-dimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, (5α , 6α , 9β , $14a\alpha$, 15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:717840 CAPLUS

DN 123:227862

TI Synthesis of saframycins. XII. Total synthesis of (-)-N-acetylsaframycin Mx 2 and its epi-(+)-enantiomer

AU Saito, Naoki; Harada, Shunji; Inouye, Izumi; Yamaguchi, Kentaro; Kubo, Akinori

CS Meiji Coll. Pharmacy, Tokyo, 154, Japan

SO Tetrahedron (1995), 51(30), 8231-46 CODEN: TETRAB; ISSN: 0040-4020

PB Pergamon

DT Journal

LA English

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The first total synthesis of (-)-N-acetylsaframycin Mx 2 I from (±)-pentacyclic amine II is described. The reaction of II with Cbz-L-alanine gave an inseparable mixture of amides III and IV (R = CO2CH2Ph). Deprotection of the Cbz group to amines followed by treatment with acetic anhydride in pyridine produced amides III and IV (R = Ac) (V). The structure of V was determined by X-ray crystallog. The conversion of III (R = Ac) to a bisquinone and subsequent stereoselective and regioselective introduction of the methoxyl group at position 5 provided VI. Finally, VI was subjected to catalytic reduction and regioselective oxidation to give I.

On

the other hand, the epi-enantiomer V was transformed to epi-(+)-I in a same four-step sequence. The specific optical rotation and the CD spectra of I and its epimer were of opposite sign. The assignment of the absolute configuration of saframycins Mx as 5S,6R,9R,14aS,15R,19S is also discussed.

IT 112995-89-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (total synthesis of saframycin Mx 2 and epimer)

RN 112995-89-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 168415-87-0 CAPLUS
CN Carbamic acid, [2-[[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]amino]-1-methyl-2-oxoethyl]-, phenylmethyl ester,
[6S-[6α,9β(R*),14aα,15α]]- (9CI) (CA INDEX NAME)

RN 168415-89-2 CAPLUS
CN Propanamide, 2-amino-N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [6S-[6α,9β(R*),14aα,15α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 168415-91-6 CAPLUS
CN Propanamide, 2-(acetylamino)-N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [6S-[6α,9β(R*),14aα,15α]]- (9CI) (CA INDEX NAME)

RN 168415-97-2 CAPLUS

CN Propanamide, 2-(acetylamino)-N-[(6,7,9,14,14a,15-hexahydro-1,4,10,13-tetrahydroxy-2,5,11-trimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [5S-[5 α ,6 α ,9 β (R*),14a α ,15 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168609-86-7 CAPLUS

CN Carbamic acid, [2-[[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]amino]-1-methyl-2-oxoethyl]-, phenylmethyl ester, [6R-[6 α ,9 β (S*),14a α ,15 α]]- (9CI) (CA INDEX NAME)

168609-88-9 CAPLUS RNCN

Propanamide, 2-amino-N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9yl) methyl] -, $[6R - [6\alpha, 9\beta(S^*), 14a\alpha, 15\alpha]] - (9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN

168609-90-3 CAPLUS
Propanamide, 2-(acetylamino)-N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-CN hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9yl) methyl] -, $[6R-[6\alpha, 9\beta(S^*), 14a\alpha, 15\alpha]]$ - (9CI) (CA INDEX NAME)

RN

168609-94-7 CAPLUS
Propanamide, 2-(acetylamino)-N-[(6,7,9,14,14a,15-hexahydro-1,4,10,13-CNtetrahydroxy-2,5,11-trimethoxy-3,12,16-trimethyl-6,15-imino-5Hisoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [5R- $[5\alpha, 6\alpha, 9\beta(S^*), 14a\alpha, 15\alpha]$] - (9CI) (CA INDEX NAME)

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ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
L4
AN
     1995:318223 CAPLUS
DN
     122:132813
     Synthesis of saframycins. VI. The useful transformation of (-)-saframycin
ΤI
     A to (-)-saframycin Mx type compound
ΑU
     Saito, Naoki; Nishida, Masayo; Kubo, Akinori
     Meiji Coll. Pharm., Tokyo, 154, Japan
CS
SO
     Chemical & Pharmaceutical Bulletin (1991), 39(5), 1343-5
     CODEN: CPBTAL; ISSN: 0009-2363
ΡВ
     Pharmaceutical Society of Japan
DT
     Journal
LA
     English
GΙ
```

AB A transformation of (-)-saframycin A I (Y1 = H) (II) to the saframycin Mx type compound III is described. Treating II with selenium oxide in acetic acid afforded (-)-saframycin G I (Y1 = OH), followed by catalytic reduction and regioselective oxidation to provide the hydroquinone III. IT 160952-79-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (transformation of saframycin A to Mx type compound) 160952-79-4 CAPLUS Propanamide, N-[(7-cyano-6,7,9,14,14a,15-hexahydro-1,4,5,10,13-RNCNpentahydroxy-2,11-dimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2b] [3] benzazocin-9-yl) methyl]-2-oxo-, [5S-(5 α , 6 α , 7 α , 9. bet $a.,14a\alpha,15\alpha)$] - (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:608305 CAPLUS

DN 115:208305

TI Synthesis of saframycins. VII. The synthesis of novel renieramycin congeners

AU Saito, Naoki; Yamauchi, Reiko; Kubo, Akinori

CS Meiji Coll. Pharm., Tokyo, 154, Japan

SO Heterocycles (1991), 32(6), 1203-14

CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 115:208305

GI

AB The marine alkaloid renieramycin congeners I (R = H, Ac, EtCO) were synthesized starting from the alc. II which was the key intermediate for saframycin B synthesis.

IT 112446-04-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-9-methanol,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
(6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 113083-38-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acylation of, with pyruvoyl chloride)
RN 113083-38-8 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
(6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112995-91-2P 136581-76-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and demethylation of)

RN 112995-91-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
acetate (ester), (6α,9β,14aα,15α)- (9CI) (CA INDEX
NAME)

Relative stereochemistry.

RN 136581-76-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,
 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
 propanoate (ester), (6α,9β,14aα,15α)- (9CI) (CA
 INDEX NAME)

IT 112446-14-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrazinolysis of)

RN 112446-14-7 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 136604-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 136604-12-1 CAPLUS

CN Carbonic acid, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl 1-methylethyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112529-60-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and partial demethylation of)

RN

112529-60-9 CAPLUS
Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-CN3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112529-59-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with phthalimide)

RN112529-59-6 CAPLUS

6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, CN 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 136581-72-1P 136656-90-1P 136656-91-2P 136656-92-3P 136656-93-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 136581-72-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, $(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, <math>[6\alpha,9\alpha(Z),14a\alpha,15\alpha]$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 136656-90-1 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1-hydroxy-2,4,10,11,13-pentamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

RN 136656-91-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, $(6,7,9,14,14a,15-\text{hexahydro-1},2,4,10,11,13-\text{hexamethoxy-3},12,16-\text{trimethyl-6},15-\text{imino-5H-isoquino}[3,2-b][3]benzazocin-9-yl)methyl ester, <math>[6\alpha,9\alpha(E),14a\alpha,15\alpha]-(9CI)$ (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 136656-92-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, $(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, <math>[6\alpha,9\beta(Z),14a\alpha,15\alpha]$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 136656-93-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b] [3]benzazocin-9-yl)methyl ester, [6 α ,9 β (E),14a α ,15 α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

IT 112529-58-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:441435 CAPLUS

DN 115:41435

ΤI Computer simulation of the binding of saframycin A to d(GATGCATC)2

ΑU Hill, G. Craig; Remers, William A.

CS Coll. Pharm., Univ. Arizona, Tucson, AZ, 85271, USA

Journal of Medicinal Chemistry (1991), 34(7), 1990-8 SO CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

English LA

AB The binding of saframycin A to the octanucleotide duplex d(GATGCATC)2 was investigated using mol. dynamics. For covalent binding at N2 of the central guanine, only the R configuration at the alkylating carbon (C7) was permitted for B DNA and the 3' direction in the minor groove was preferred by 11 kcal/mol. The dihydroquinone form of saframycin A gave stronger binding than the quinone, in agreement with the literature. Addition of solvent and counterions made no significant change in the geometry of the preferred model. The proposed mechanism of DNA alkylation, involving iminium ion intermediates from the dihydroquinone or quinone, was investigated by modeling these species. They gave models with good net binding enthalpies, and C7 was in close proximity to N2 of guanine. The noncovalent binding of saframycin A and its dihydroquinone in the vicinity og guanine also was favorable in the 3' direction.

IT 133966-18-4

RL: BIOL (Biological study)

(binding of, to octanucleotide duplex, mol. modeling of)

RN

133966-18-4 CAPLUS
Propanamide, N-[(7-cyano-6,7,9,14,14a,15-hexahydro-1,4,10,13-tetrahydroxy-CN 2,11-dimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2b] [3]benzazocin-9-yl)methyl]-2-oxo-, [6S-(6 α ,7 α ,9 β ,14a.al pha., 15α)] - (9CI) (CA INDEX NAME)

L4ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN ΑN 1991:102523 CAPLUS DN 114:102523 ΤI A stereocontrolled total synthesis of (\pm) -renieramycin A ΑU Fukuyama, Tohru; Linton, Steven D.; Tun, Min Min CS Dep. Chem., Rice Univ., Houston, TX, 77251, USA SO Tetrahedron Letters (1990), 31(42), 5989-92 CODEN: TELEAY; ISSN: 0040-4039 DT Journal LA English GI

Ι

CN 2-Butenoic acid, 2-methyl-, $(6,7,9,14,14a,15-hexahydro-1,5,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, <math>[5\alpha,6\alpha,9\alpha(Z),14a.alpha.,15\alpha]$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

IT 132277-62-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, crystal structure, and oxidation of)

RN 132277-62-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, $(6,7,9,14,14a,15-\text{hexahydro-1},5,10-\text{trihydroxy-2},4,11,13-\text{tetramethoxy-3},12,16-\text{trimethyl-6},15-\text{imino-5H-isoquino}[3,2-b][3]benzazocin-9-yl)methyl ester, <math>[5\alpha,6\alpha,9\beta(Z),14a.alpha$.,15 α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

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L4
     ANSWER 16 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1990:406006 CAPLUS
DN
     113:6006
TI
     Total synthesis of (\pm)-saframycin A
ΑU
     Fukuyama, Tohru; Yang, Lihu; Ajeck, Karen L.; Sachleben, Richard A.
CS
     Dep. Chem., Rice Univ., Houston, TX, 77251, USA
SO
     Journal of the American Chemical Society (1990), 112(9), 3712-13
     CODEN: JACSAT; ISSN: 0002-7863
DT
     Journal
     English
LA
os
     CASREACT 113:6006
GI
```

A highly efficient total synthesis of (\pm) -saframycin A (I) is reported. AΒ The dimeric nature of this unique bisquinone antitumor antibiotic allowed the use of the readily available, C2-sym. N,N'-diacetyl-2,5piperazinedione (II) as the starting material. Condensation of II with the aldehyde III to form the arylidenepiperazinedione clearly introduced the nonsym. element needed to construct the bicyclic ring system. The present synthetic route is suitable for a large scale preparation of I and its analogs, giving 8.7% overall yield from II. IT 127103-59-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oxidation of) 127103-59-7 CAPLUS
Propanamide, N-[(7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-RNCN

Propanamide, N-[(7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha,7\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 127103-58-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, deblocking and acylation of)

RN 127103-58-6 CAPLUS

CN Carbamic acid, [(7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, 1,1-dimethylethyl ester, $(6\alpha,7\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

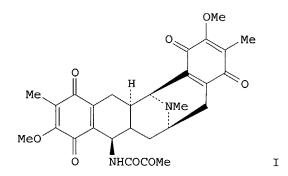
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ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
L4
     1989:55972 CAPLUS
ΑN
DN
     Manufacture of antitumor antibiotic saframycins with Myxococcus
TI
     Gesellschaft fuer Biotechnologische Forschung m.b.H., Switz.
PA
SO
     Jpn. Kokai Tokkyo Koho, 19 pp.
     CODEN: JKXXAF
DT
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                           APPLICATION NO. DATE
PI
     JP 63049092
                      A2
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                                           JP 1987-202012
                                                            19870814
     EP 262085
                      A1
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     AU 605783
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                                                            19900907
     AU 628643
                       B2
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PRAI CH 1986-3294
                            19860815
    MARPAT 110:55972
OS
GT
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Antitumor antibiotic saframycin I (R1 = H, OH; R2 = H, acyl; A, B = C:O, C-OH; if A, B = C:O, the middle section of each of the broken lines would be double bonds; if A, B = C-OH, the 2 sides of each of the broken lines would be double bonds) is manufactured by fermentation with Myxococcus. Its pharmaceutical application is also disclosed. M. xanthus Mx x48 was cultivated in a 700 mL MD11.m medium with agitation and aeration for 50 h. I, predominantly I-Mx 1 and I-Mx 2, 700 mg were recovered from the culture fluid.
- IT 116925-62-3P
 RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
 (Preparation)

(manufacture of, with Myxococcus xanthus, as tumor inhibitor)

- RN 116925-62-3 CAPLUS
- CN Propanamide, 2-amino-N-[(6,7,9,14,14a,15-hexahydro-1,4,7,10,13-pentahydroxy-2,5,11-trimethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [5S-[5 α ,6 β ,7 α ,9 β (R*),14a α ,15 β]- (9CI) (CA INDEX NAME)

ANSWER 18 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN L4AN 1988:510118 CAPLUS DN 109:110118 Stereoselective total synthesis of (\pm) -saframycin B TIKubo, Akinori; Saito, Naoki; Yamato, Hidekazu; Masubuchi, Kazunao; ΑU Nakamura, Madoka CS Meiji Coll. Pharm., Tokyo, 154, Japan SO Journal of Organic Chemistry (1988), 53(18), 4295-310 CODEN: JOCEAH; ISSN: 0022-3263 DTJournal LA English OS CASREACT 109:110118 GT



Relative stereochemistry.

IT 113083-37-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrazinolysis of)

113083-37-7 CAPLUS RN

CN1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9yl) methyl] -, $(6\alpha, 9\beta, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-03-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidative demethylation of)

RN

112446-03-4 CAPLUS
Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-CN3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha, 9\beta, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 115678-29-0P 115678-31-4P

Relative stereochemistry.

RN 115678-31-4 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,4-dihydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, monomethyl ether, $(6\alpha,9\beta,14a\alpha,15.alpha.)$ - (9CI) (CA INDEX NAME)

CM 1

CRN 115678-29-0 CMF C30 H39 N3 O8

CM 2

CRN 67-56-1 CMF C H4 O

 $_{\rm H_3C-OH}$

IT 112446-04-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with phthalimide)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112995-89-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with pyruvoyl chloride)
RN 112995-89-8 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
(6α,9β,14aα,15β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112529-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and transesterification of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3] benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 115794-03-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 115794-03-1 CAPLUS

CN Propanamide, N-[[1(or 4)-(acetyloxy)-6,7,9,14,14a,15-hexahydro-2,4,10,11,13(or 1,2,10,11,13)-pentamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl]-2-oxo-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

CM 1

CRN 115678-29-0 CMF C30 H39 N3 O8

Relative stereochemistry.

CM 2

CRN 67-56-1 CMF C H4 O

н3С-он

CM 3

CRN 64-19-7 CMF C2 H4 O2

L4 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:473253 CAPLUS

DN 109:73253

TI Preparation of 6,15-iminoisoquino[3,2-b][3]benzazocine derivatives as intermediates for an antitumor agent saframycin B

IN Kubo, Yotoku; Saito, Naoki

PA Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DT Patent

LA. Japanese

FAN.CNT 1

1710. CN1 1					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 63002991	A2	19880107	JP 1986-144916	19860623
PRAI	JP 1986-144916		19860623		
os	MARPAT 109:73253				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Isoquinolines I (R = CH2OH, CH2NH2, phthaloylmethyl) (II) are prepared from diazabicyclononane III. A mixture of III and K2CO3 in BuOH was treated with OHCCO2Bu at room temperature for 67 h and the concentrated reaction mixture was stirred

in CF3CO2H at ice-cooled temperature for 1 h to give 70.2% isoquinoline IV, which was isomerized by treatment with Hg(OAc)2 in AcOH and then H2S(g), followed by NaBH4 treatment of the product in EtOH in the presence of NaHCO3 to give 70.6% I (R = CO2Bu) (V). A mixture of V and LiAlH4 in THF was refluxed for 2 h to afford 76.8% I (R = CH2OH), which was converted to saframycin B in 4 steps.

IT 115510-17-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and LAH reduction of, in preparation of saframycin B)

RN 115510-17-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
butyl ester, [6R-(6α,9α,14aβ,15α)]- (9CI) (CA
INDEX NAME)

IT 115510-16-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and isomerization of, in preparation of saframycin B)

RN 115510-16-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $[6R-(6\alpha,9\beta,14a\beta,15\alpha)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

IT 115510-18-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of, saframycin B from)

RN

115510-18-4 CAPLUS
Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-CN 3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-0x0-, $[6R-(6\alpha, 9\alpha, 14a\beta, 15\alpha)]$ - (9CI) (CA INDEX NAME)

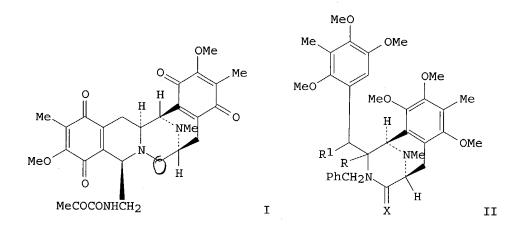
Absolute stereochemistry.

RN 115510-14-0 CAPLUS CN 1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, [6R-(6α,9α,14aβ,15α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 115510-15-1 CAPLUS CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, $[6R-(6\alpha,9\alpha,14a\beta,15\alpha)]-(9CI)$ (CA INDEX NAME)

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ANSWER 20 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
T.4
AN
     1988:112030 CAPLUS
     108:112030
DN
TI
     Synthesis of saframycins.
                                I. Total synthesis of (\pm)-saframycin B and
     its congeners
     Kubo, Akinori; Saito, Naoki; Yamauchi, Reiko; Sakai, Shinichiro
ΑU
CS
     Meiji Coll. Pharm., Tokyo, 154, Japan
SO
     Chemical & Pharmaceutical Bulletin (1987), 35(5), 2158-61
     CODEN: CPBTAL; ISSN: 0009-2363
DТ
     Journal
LA
     English
OS
     CASREACT 108:112030
GT
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The total synthesis of saframycin B (I) was achieved from tricyclic lactam AB II (RR1 = bond; X = 0). The key step is the stereoselective intramol. cyclization of the amino acetal II (R = R1 = H; X = H2). The structure of a pentacyclic intermediate was confirmed by x-ray crystallog. 112995-89-8P 113083-38-8P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and acylation of, with pyruvoyl chloride) RN112995-89-8 CAPLUS 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine, CN6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, $(6\alpha, 9\beta, 14a\alpha, 15\beta)$ - (9CI) (CA INDEX NAME)

RN 113083-38-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanamine, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-10-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, ethyl ester, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112995-91-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and demethylation of)

RN 112995-91-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3] benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, acetate (ester), $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112529-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and epimerization of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112446-14-7P 113083-37-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrazinolysis of)

RN 112446-14-7 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 113083-37-7 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112446-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 112446-03-4 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-04-5P 112529-59-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with phthalimide)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-9-methanol,
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,
(6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 112529-59-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-05-6P

 $\mbox{RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) } \\$

(preparation and reduction of)

RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112995-90-1P

RN 112995-90-1 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,1,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:55713 CAPLUS

DN 108:55713

TI Studies on the total synthesis of saframycin B

AU Kobo, Akiyoshi; Saito, Naoki; Yamato, Hidekazu; Nakamura, Madoka

CS Meiji Coll. Pharm., Japan

SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1986), 28th, 465-72 CODEN: TYKYDS

DT Journal

LA Japanese

GΙ

II

III

AB Saframycin B (I) which is an antitumor antibiotic, produced by Streptomyces lavendulae were prepared The preparation of safaramycin B intermediate II was reviewed. II was converted into the pentacyclic compound III in 10 steps. Oxidation of III with 10N HNO3 afforded I in 1% yield. The yield of I was raised to 41% by treatment with BBr3 at -78° followed by 10N HNO3.

IT 112446-10-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, ethyl ester, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112529-59-6P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methylation of)

RN 112529-59-6 CAPLUS

CN6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidative demethylation of)

RN

112446-03-4 CAPLUS
Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-CN3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha, 9\beta, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112446-16-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 112446-16-9 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1-hydroxy-2,4,10,11,13-pentamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-11-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with azide)

RN 112446-11-4 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,

methanesulfonate (ester), $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\beta,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-13-6P 112529-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 112446-13-6 CAPLUS

CN Acetamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

RN 112529-60-9 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha, 9\alpha, 14a\alpha, 15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112446-14-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, hydrazinolysis, and acylation of)

RN 112446-14-7 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[(6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112446-04-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, reaction with phthalimide, hydrazinolysis, and acylation of)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 112529-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, reduction, and isomerization of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b] [3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

IT 112446-12-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, reduction, and N-acetylation of)

RN 112446-12-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine, 9-(azidomethyl)-6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, $(6\alpha,9\alpha,14a\alpha,15\alpha)$ - (9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1982:544641 CAPLUS

DN 97:144641

TI Stereocontrolled total synthesis of (±)-saframycin B

AU Fukuyama, Tohru; Sachleben, Richard A.

CS Dep. Chem., Rice Univ., Houston, TX, 77251, USA

SO Journal of the American Chemical Society (1982), 104(18), 4957-8 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The first total synthesis of a novel antibiotic, (±)-saframycin B (I) is reported. The benzobicyclo[3.3.1] system II (R = CO2CH2Ph) was constructed from a readily available, diastereomeric mixture of amino acid derivs. III in three steps in 74% yield. Conversion of II to the pentacyclic compound IV was carried out in a six-step sequence in 41% overall yield. Oxidation of IV with ceric ammonium nitrate gave 37% I.

IT 82638-80-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 82638-80-0 CAPLUS

CN Propanamide, N-[(6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-2-oxo-, $(6\alpha,9\alpha,14a\beta,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 82660-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 82660-66-0 CAPLUS

CN Carbamic acid, [(6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-

tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, phenylmethyl ester, $(6\alpha,9\beta,14a\beta,15\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 82638-79-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, deblocking, and acylation of)

RN 82638-79-7 CAPLUS

CN Carbamic acid, [(6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl]-, phenylmethyl ester, $(6\alpha,9\alpha,14a\beta,15\alpha)$ - (9CI) (CA INDEX NAME)

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